AME 60636
Prof. J. M. Powers
Homework 6
Due: Monday, 2 October 2006

1. Consider a reaction mechanism for the combustion of H_2 with O_2 as given by Powers and Paolucci [1] in their Table 1. This is available on the links section of the course web page. Consider combustion in a fixed volume which is a cube whose side is of length 200 mm. The gas has initial mole fractions of $y_{H_2} = 0.3$, $y_{O_2} = 0.15$, $y_{N_2} = 0.55$, and an initial pressure and temperature of 0.1 MPa and 1000 K. Take N_2 to be an inert diluent.

   For adiabatic, isochoric combustion, determine the variation of all species concentrations, temperature, pressure, and time scales of reaction as functions of time; give computer-generated plots on logarithmic scales. Plot all species concentrations on a single plot. Plot all time scales on a single plot. Plot the relative error in energy $\frac{u(t)-u(0)}{u(0)}$, and the relative error in moles for each atom versus time. You will need to computationally calculate the Jacobian matrix and associated eigenvalues. IMSL or lapack subroutines are available in Fortran to enable this calculation. It is also possible to write your own software.

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[1] Powers, J. M., and Paolucci, S., 2005, "Accurate Spatial Resultion Estimates for Reactive Supersonic Flow with Detailed Chemistry," *AIAA Journal*, Vol. 43, No. 5, pp. 1088-1099.